Vortex nucleation in rotating Bose-Einstein condensates

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We study the formation and stability of a single vortex state in a weakly-interacting Bose-Einstein condensate that is confined in a rotating harmonic potential. Our results are consistent with the fact that any single off-center vortex is unstable. Furthermore, a vortex state located at the center of the cloud first becomes locally stable as the rotational frequency increases. Finally our study implies the existence of hysteresis effects.

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When rotated, a superfluid forms quantized vortex states. Numerous studies have examined in the past vortices in the traditional superfluid liquid Helium IV. Recently in some remarkable experiments vortices have also been created and observed in vapors of trapped ultracold atoms [1, 2, 3, 4].

One of the basic questions in atomic systems is the formation and stability of vortex states. Because of the confinement (which is typically harmonic), there is a number of differences as compared to homogeneous superfluids. For example, the energy spectrum is discreet, the density is inhomogeneous and finally for harmonic confinement the frequency of rotation of the gas is limited by the trap frequency.

Many studies have examined the physics of vortices in trapped gases [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]. The basic picture is that above a critical frequency of rotation of the trap, one vortex state forms in the gas, while as the rotational frequency increases further, more vortices enter the cloud, eventually forming an array. One of the most fundamental and important questions is thus the way that the first vortex state forms.

In the present study we develop a method which allows us to examine this problem in the limit of weak interactions, where the typical atom-atom interaction energy is smaller than the oscillator quantum of energy and one can restrict himself to the subspace of states in the lowest Landau level. In this limit the gas has a very peculiar property when the angular momentum per atom ranges between zero and unity, as the interaction energy scales linearly with the angular momentum [14, 17, 18, 19, 20], just like as in an ideal gas. This is an exact result within the lowest Landau level subspace of states.

The linear behavior of the spectrum has important implications on the rotational properties of the gas, as at a critical frequency of rotation which is smaller than the trap frequency by a (small) amount that is proportional to the ratio between the interaction energy and the oscillator energy, the gas is predicted to undergo a discontinuous phase transition from a non-rotating state to a state with one vortex at the center of the trap [14].

However, as we show below, one needs to be careful with the effect of the truncation to the lowest Landau level wavefunctions. In the present study, using second-order perturbation theory we calculate the energy of the system to second order, where the energy no longer increases linearly with the angular momentum. From the derived dispersion relation we then examine the energy in the rotating frame, finding that the gas exhibits a non trivial and interesting behavior as function of the rotational frequency of the trap Ω.

Our study suggests that any single off-center vortex state is unstable. Furthermore, a vortex state that is located at the center of the cloud first becomes locally stable. We also predict that the gas comes to rest at a smaller Ω than the one where rotation sets in (see Fig. 1), and the system exhibits hysteresis [15], which is a general characteristic of first-order phase transitions. The graphs in Fig. 1 show schematically the energy of the gas in the rotating frame for certain physically-relevant rotational frequencies which we calculate below.

In our model we consider atoms interacting via a short-range effective interaction,

$$V_{\rm int} = U_0 \sum_{i\neq j} \delta(\mathbf{r}_i - \mathbf{r}_j)/2. \qquad (1)$$

Here $U_0 = 4\pi\hbar^2 a/M$ is the strength of the effective two-body interaction, where a is the scattering length for elastic atom-atom collisions and M is the atom mass. We also consider a harmonic trapping potential of the form

$$V(\rho, z) = M\omega^2(\rho^2 + \lambda z^2)/2, \qquad (2)$$

where ρ and z are cylindrical polar coordinates, ω is the oscillator frequency, and λ is a dimensionless constant ($\hbar = M = \omega = 1$ from now on.)

We consider weak interactions and strong confinement along the z axis, which is taken to be the axis of rotation. For weak interactions the corresponding dimensionless quantity is $\gamma = Na/d_z$ which is our expansion parameter as it is assumed to be much smaller than unity. Here N is the total number of atoms and d_z is the oscillator length along the axis of rotation. In this limit one can work within the subspace of the nodeless ($n = 0$) eigenfunctions of the two dimensional harmonic oscillator,

$$\psi_{n,m}(\rho,\phi) = \sqrt{\frac{n!}{\pi(n+|m|)!}}\,\rho^{|m|}e^{im\phi}L_n^m(\rho^2)e^{-\rho^2/2}, \quad (3)$$

where n is the number of radial excitations, m is the quantum number of the angular momentum, and L_n^m are

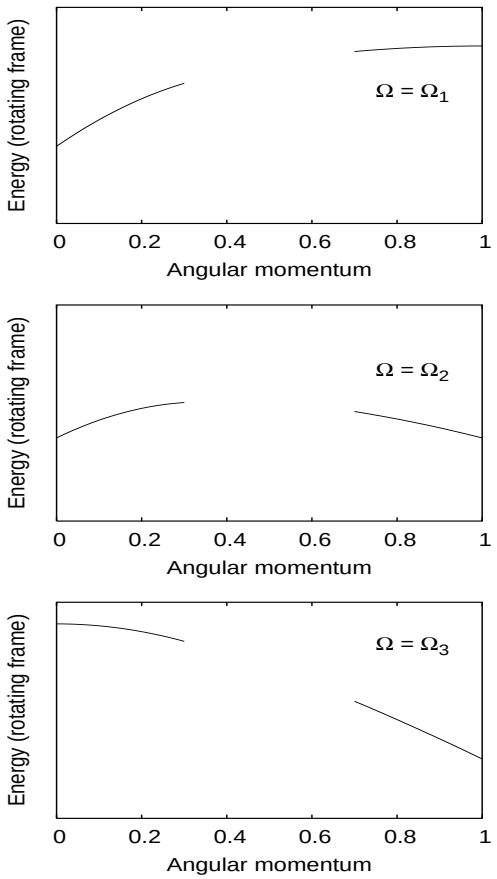

FIG. 1: Schematic diagram which shows the energy of the gas in the rotating frame as function of the angular momentum per atom l for different frequencies of rotation Ω. On the top graph, for $\Omega = \Omega_1$, the derivative of the energy at $l = 1$ vanishes. For $\Omega = \Omega_2$ the energy at $l = 0$ equals that at $l = 1$. Finally, for $\Omega = \Omega_3$ the derivative of the energy at $l = 0$ vanishes. Our study shows that $\Omega_1 < \Omega_2 < \Omega_3$, and also that the energy bents downward at both $l = 0$ and $l = 1$. All these observations have crucial consequences on the formation and stability of a single vortex state.

the associated Laguerre polynomials. More specifically, the basis states are $\psi_{0,m}(\rho,\phi) = \rho^{|m|}e^{im\phi}e^{-\rho^2/2}/\sqrt{\pi|m|!}$.

The strong confinement along the axis of rotation, $\lambda \gg 1$, implies that the cloud is in its lowest state of motion along this axis, and the problem thus becomes effectively two dimensional, as the degrees of freedom along the z axis are frozen out. Therefore, the order parameter $\Psi(\mathbf{r})$ can be expanded in the product states $\Psi_{0,m}(\mathbf{r}) = \psi_{0,m}(\rho,\phi)\,\phi_0(z)$, where $\phi_0(z)$ is the ground state of the one dimensional harmonic oscillator.

Under the above conditions, as shown initially by Bertsch and Papenbrock [17] using numerical diagonalization, the interaction energy of the gas in the lowest state is, for $2 \le L \le N$,

$$\mathcal{E}_{L,N} = \gamma(N - L/2 - 1)/\sqrt{2\pi}, \tag{4}$$

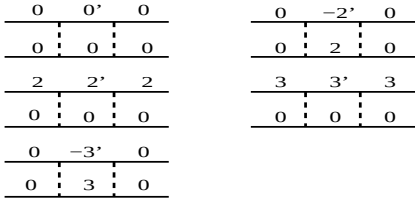

FIG. 2: The five diagrams which contribute to the energy of the gas to order γ^2 and up to $l^{3/2}$, for $1 \ll L \ll N$. The unprimed (primed) numbers denote the angular momentum m of the states with zero (any nonzero) radial excitations, $n = 0$ ($n \ge 1$). For the states with $m < 0$, n can also be zero. The dotted lines denote the interaction.

where L is the total angular momentum, and therefore it varies linearly with L. References [19] have shown analytically that this equation is *exact* to first order in γ.

Therefore, if $F = E - L\Omega$ is the total energy of the gas in the rotating frame, where $E = L + \mathcal{E}_{L,N}$ is the total energy in the rest frame then to first order in γ (henceforth the energy is measured with respect to the energy of the lowest state and terms of order $1/N$ are neglected), $F/N = (1 - \gamma/2\sqrt{2\pi} - \Omega)\,l$, where $l = L/N$. The above equation implies that the critical frequency for rotation is

$$\Omega_c^{(1)} = 1 - \gamma/2\sqrt{2\pi}. \tag{5}$$

At this value of Ω Butts and Rokhsar [14] predict that the gas undergoes a discontinuous transition from a non rotating state to a state with a vortex located at the center of the trap. In the present study we calculate the energy to next order for $0 \le l \le 1$ examining how this picture is modified. On the other hand, for $l > 1$ where more than one vortices are present, calculation of the energy to lowest order in γ suffices to determine their stability.

We use now second-order perturbation theory to calculate the interaction energy to next order, i.e., to γ^2. In a similar method Ref. [20] has calculated the low-lying excitations of the system in the limit of low angular momentum. In our study we use the results of Ref. [18] which has studied both regimes of low ($1 \ll L \ll N$) and high ($1 \ll N - L \ll N$) angular momentum. Starting with $1 \ll L \ll N$, since we need both the slope, as well as the curvature of the energy (which is given by a term of order $l^{3/2}$ in this case), the order parameter is, up to the desired order,

$$\Psi = c_0\Psi_{0,0} + c_2\Psi_{0,2} + c_3\Psi_{0,3}, \tag{6}$$

where $|c_0|^2 = 1 - l/2 + l^{3/2}/3$, $|c_2|^2 = l/2 - l^{3/2}$, and $|c_3|^2 = 2l^{3/2}/3$. The five diagrams which contribute to the energy to second order in γ and up to $l^{3/2}$ are shown in Fig. 2. For example, the contribution of the top left diagram to the energy per particle is equal to

$$\sum_{n=1}^{\infty} \frac{|\langle\Psi_{0,0},\Psi_{0,0}|V_{\rm int}|\Psi_{0,0},\Psi_{n,0}\rangle|^2}{N(\epsilon_{0,0}-\epsilon_{n,0})} = \sum_{n=1}^{\infty} \frac{|I_{0,0}^{0,n}|^2 N_0^3 U_0^2}{N(\epsilon_{0,0}-\epsilon_{n,0})}$$

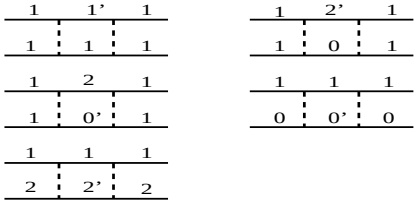

FIG. 3: The five diagrams which contribute to the energy of the gas to order γ^2 and up to l^2, for $1 \ll N - L \ll N$.

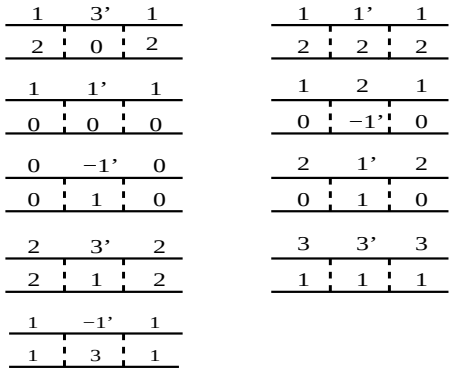

FIG. 4: The nine diagrams which contribute to the energy of the gas to order γ^2 and to l^2, for $1 \ll N - L \ll N$.

$$= -(1 - l/2 + l^{3/2}/3)^3 (NU_0)^2 \sum_{n=1}^{\infty} \frac{|I_{0,0}^{0,n}|^2}{\epsilon_{n,0} - \epsilon_{0,0}}, \quad (7)$$

where $I_{0,0}^{0,n} = \int \Psi_{0,0}^* \Psi_{0,0}^* \Psi_{0,0} \Psi_{n,0}\, d\mathbf{r}$ is the overlap integral between the corresponding states. This always involves three states with zero radial excitations and one state with n radial excitation(s). Also $\epsilon_{n,m} = 2n + |m| + 1 + \lambda/2$ is the eigenenergy of the states $\Psi_{n,m}(\mathbf{r}) = \psi_{n,m}(\rho, \phi)\phi_0(z)$ and $N_0 = N|c_0|^2$ is the occupancy of the state $\Psi_{0,0}$. In Eq. (7) there is a factor of $1/2$ from the interaction [Eq. (1)] that is cancelled by a factor of 2 that comes from the symmetrization of the wavefunction.

The sum in Eq. (7) is over all the excited states with $m = 0$ and $n \geq 1$ (in other cases where intermediate states with negative values of m are involved, $n \geq 0$.) However, the series converges rapidly because of the overlap integrals which decrease with increasing n. Considering the first fifteen excited states, $n = 1, \ldots, 15$ we find that

$$E/N \approx \left(1 - \gamma/2\sqrt{2\pi}\right) l - \left(0.0916 - 0.0883\, l + 0.0156\, l^{3/2}\right) \gamma^2. \quad (8)$$

As a final step we express E/N as function of the expectation value of the angular momentum per particle $\langle l \rangle \equiv \langle \tilde{\Psi} | \hat{L} | \tilde{\Psi} \rangle / \langle \tilde{\Psi} | \tilde{\Psi} \rangle$. Here $\tilde{\Psi} = \sum_m c_m \tilde{\Psi}_m$, with $\tilde{\Psi}_m = \Psi_{0,m} + \gamma \sum_{n \neq 0} d_{n,m} \Psi_{n,m}$ being the perturbed basis states. The corrections of order γ in the basis states introduce a correction of order γ^2 in $\langle l \rangle - l$.

To calculate $\langle l \rangle$ we start from the Gross-Pitaevskii equation and make use of the orthogonality between the states $\Psi_{n,m}$ finding $d_{n,m} = -2\pi \int |\Psi_{0,m}|^2 \Psi_{0,m} \Psi_{n,m}^*\, d\mathbf{r}/n$. This formula implies that $\langle l \rangle = l[1 - 0.0405\,\gamma^2 - 0.0018\,\gamma^2\, l^{1/2}]$, or $l = \langle l \rangle [1 + 0.0405\,\gamma^2 + 0.0018\,\gamma^2 \langle l \rangle^{1/2}]$. Combining this result with Eq. (8) we find

$$E/N \approx \left(1 - \gamma/2\sqrt{2\pi}\right) \langle l \rangle - \left(0.0916 - 0.1288\, \langle l \rangle + 0.0138\, \langle l \rangle^{3/2}\right) \gamma^2. \quad (9)$$

From Eq. (9) we conclude that the critical frequency of rotation is, to order γ^2,

$$\Omega_c^{(2)} \equiv \Omega_3 = 1 - \gamma/2\sqrt{2\pi} + 0.1288\,\gamma^2 + \mathcal{O}(\gamma^3). \quad (10)$$

Also E/N (as well as F/N) has a downward curvature.

Following a similar method we perform the same analysis for $1 \ll N - L \ll N$. There is no term of order $\tilde{l}^{3/2}$ in this case and the two leading terms are of order $\tilde{l}$ and $\tilde{l}^2$, where $\tilde{l} = 1 - l$. The corresponding order parameter is [18]

$$\Psi = c_0 \Psi_{0,0} + c_1 \Psi_{0,1} + c_2 \Psi_{0,2} + c_3 \Psi_{0,3}, \quad (11)$$

where $|c_0|^2 = 2\tilde{l} - 3\tilde{l}^2/2$, $|c_1|^2 = 1 - 3\tilde{l} + 27\tilde{l}^2/8$, $|c_2|^2 = \tilde{l} - 9\tilde{l}^2/4$, and $|c_3|^2 = 3\tilde{l}^2/8$.

The five diagrams which contribute to the interaction energy linearly and quadratically in $\tilde{l}$ are shown in Fig. 3, while the ones in Fig. 4 contribute only quadratically. Again, considering the first fifteen excited states we find

$$E/N \approx \left(1 - \gamma/2\sqrt{2\pi}\right)(1 - \tilde{l}) - \left(0.0111 + 0.1024\,\tilde{l} + 0.7654\,\tilde{l}^2\right) \gamma^2. \quad (12)$$

In this case $\langle \tilde{l} \rangle = \tilde{l}[1 + 0.0780\,\gamma^2 - 0.0811\,\tilde{l}\,\gamma^2]$, or $\tilde{l} = \langle \tilde{l} \rangle [1 - 0.0780\,\gamma^2 + 0.0811\,\langle \tilde{l} \rangle\, \gamma^2]$. The energy, expressed as function of $\langle \tilde{l} \rangle$ is therefore

$$E/N \approx \left(1 - \gamma/2\sqrt{2\pi}\right)\left(1 - \langle \tilde{l} \rangle\right) - \left(0.0111 + 0.0244\,\langle \tilde{l} \rangle + 0.8465\,\langle \tilde{l} \rangle^2\right) \gamma^2. \quad (13)$$

The frequency at which the derivative vanishes is thus

$$\Omega_1 = 1 - \gamma/2\sqrt{2\pi} + 0.0244\,\gamma^2 + \mathcal{O}(\gamma^3). \quad (14)$$

Again, E/N (and F/N) has a downward curvature.

Finally, another relevant frequency of rotation is the one where the energy in the rotating frame for $\langle l \rangle = 0$ equals that for $\langle l \rangle = 1$, and this turns out to be

$$\Omega_2 = 1 - \gamma/2\sqrt{2\pi} + 0.0805\,\gamma^2 + \mathcal{O}(\gamma^3), \quad (15)$$

in agreement with Ref. [21].

Having calculated the energy as function of the angular momentum in the two limiting cases, we can extract valuable information about the formation and stability of a single vortex state. Since our Hamiltonian is rotationally invariant, it commutes with the angular momentum and therefore the angular momentum is a good quantum number. In that respect, any configuration is stable, however the interesting question is the stability against weak perturbations.

For example, in the presence of a small thermal component in the gas which interacts with the condensate exchanging angular momentum and energy with it, a vortex state is stable/metastable as long as its energy in the rotating frame has an absolute/local minimum [22]. In the limit of weak interactions that we consider here, the energy is dominated by the oscillator energy and the energy barriers are small. As a result, these systems cannot support persistent currents [i.e., $F(l)$ does not have any metastable minimum at any $l \neq 0$ when $\Omega = 0$]. Still, when $\Omega \neq 0$, $F(l)$ develops in principle local minima and in what follows, we consider a vortex state as a stable configuration provided that $F(l)$ has a local/absolute minimum (henceforth l is to be identified as $\langle l \rangle$).

The angular momentum plotted on the horizontal axis of Fig. 1 is directly related to the position of the vortex, since for an off-center vortex state $0 < l < 1$ [23]. Therefore, as l increases in Fig. 1 the vortex moves from an infinite distance away from the trap ($l = 0$) to its center ($l = 1$).

Our results here are exact for weak interactions and for values of the angular momentum close to zero and unity. Still, our expansion strongly suggests that the schematic form of $F(l)$ shown in Fig. 1 extends over all the intermediate values of the angular momentum, without any local minima in between.

As shown in Fig. 1 for any frequency Ω between Ω_1 and Ω_2, $F(l)$ has a local minimum at $l = 1$. In other words a vortex that is located at the center of the trap first becomes stable locally with increasing Ω. This behavior is qualitatively the same as in Ref. [16] where the opposite limit of strong interaction was considered.

According to our study, if one first cools down below the condensation temperature and then rotates, the gas will undergo a discontinuous transition from a non-rotating state to a state with a vortex in the middle of the cloud for $\Omega = \Omega_3$. In the reverse process as Ω decreases, the gas will make a discontinuous transition from $l = 1$ to $l = 0$ at an $\Omega = \Omega_1$, with $\Omega_1 < \Omega_3$.

In the other physically-relevant situation, if one first rotates with some $\Omega = \Omega_0$ and then cools down below the condensation temperature, the gas may actually reach the state with a (stable) centered vortex for any value of Ω_0 between Ω_1 and Ω_3.

It is crucial to mention that the slope of $F(l)$ increases discontinuously as one crosses the point $l = 1$ by an amount of order γ, equal to $11\gamma/32\sqrt{2\pi}$ [18] (not shown in Fig. 1). This fact guarantees that $F(l)$ increases for $l \gtrsim 1$ for all the values of Ω considered above.

To summarize, the spectrum of a weakly-interacting Bose-Einstein condensate that is confined in a rotating harmonic trap implies that a vortex state located at the center of the cloud becomes first locally stable. On the other hand, any single off-center vortex is unstable. Finally we predict hysteresis as the frequency of rotation of the trap varies.

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